

## STN Structure Search

10/539, 151

02/19/2007

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FILE 'HOME' ENTERED AT 10:29:51 ON 19 FEB 2007

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COST IN U.S. DOLLARS  
  
FULL ESTIMATED COST

SINCE FILE ENTRY	TOTAL SESSION
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STRUCTURE FILE UPDATES: 18 FEB 2007 HIGHEST RN 921759-52-6  
DICTIONARY FILE UPDATES: 18 FEB 2007 HIGHEST RN 921759-52-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 30, 2006

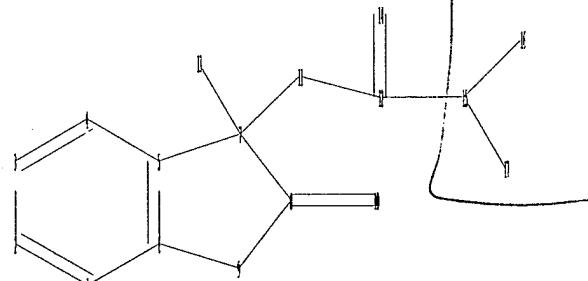
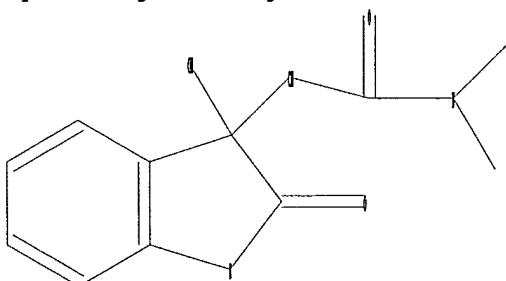
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<http://www.cas.org/ONLINE/UG/reqprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10539151\formula IIa.str



ring } chain

chain nodes :

Searched by Jason M. Nolan, Ph.D.

Page 2

```

ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
15 16 17
chain bonds :
7-11 7-13 8-10 11-12 12-14 12-15
ring/chain bonds :
15-16 15-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 7-13 8-9 8-10 12-14 12-15 15-16 15-17
exact bonds :
7-11 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

Match level :

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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS

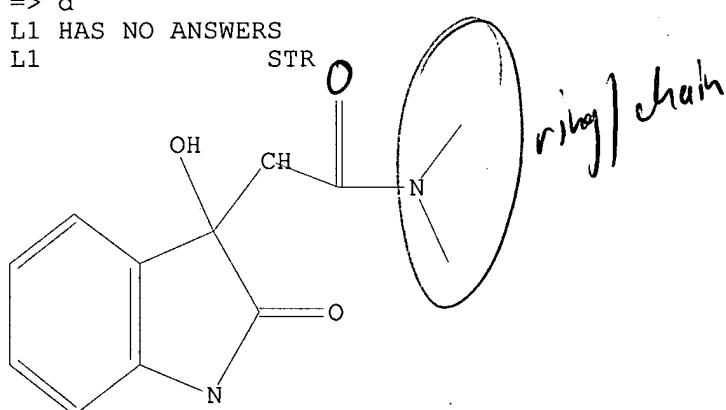
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L1        STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1



Structure attributes must be viewed using STN Express query preparation.

=> s 11 full

FULL SEARCH INITIATED 10:30:14 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 782 TO ITERATE

100.0% PROCESSED      782 ITERATIONS  
SEARCH TIME: 00.00.01

L2        11 SEA SSS FUL L1

=> fil caplus  
COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
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11 ANSWERS

10/539,151

02/19/2007

FULL ESTIMATED COST 172.10 172.31

FILE 'CAPLUS' ENTERED AT 10:30:34 ON 19 FEB 2007  
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FILE COVERS 1907 - 19 Feb 2007 VOL 146 ISS 9  
FILE LAST UPDATED: 18 Feb 2007 (20070218/ED)

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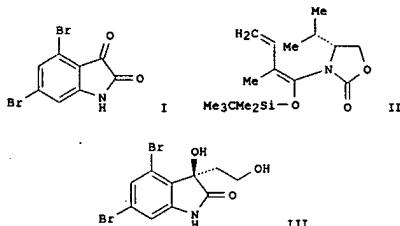
<http://www.cas.org/infopolicy.html>

=> s 12  
L3

3 L2

=> d ibib abs hitstr 1-3

L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2006:49644 CAPLUS  
 DOCUMENT NUMBER: 144:292911  
 TITLE: Enantioselective Total Synthesis of Convolutamydines B  
 AUTHOR(S): and E Nakamura, Tomoaki; Shirokawa, Shinichi; Hosokawa, Seiji; Nakazaki, Atsuo; Kobayashi, Susumu  
 CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Tokyo University of Science (RIKADAI), Chiba, 278-8510, Japan  
 SOURCE: Organic Letters (2006), 8(4), 677-679  
 CODEN: ORLETF; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:292911  
 GI



AB The first enantioselective total synthesis of convolutamydines B and E has been achieved using our vinylogous Mukaiyama aldol reaction. The synthesis features highly diastereoselective vinylogous Mukaiyama aldol reaction with isatin instead of aldehydes to construct a chiral center of convolutamydines. Thus, isatin I was reacted with N,O-acetal II to give the aldol adduct, which was transformed in several steps to (R)-convolutamydine E III. Addnl., the absolute configuration of natural convolutamydine B has been determined as R by its CD spectrum.  
 IT 879123-17-8  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (asym. total synthesis of convolutamydines B and E via diastereoselective vinylogous Mukaiyama aldol of isatin derivative)  
 RN 879123-17-8 CAPLUS  
 CN 2-Oxazolidinone, 3-[(2,3-dihydro-3-hydroxy-2-oxo-1H-indol-3-yl)acetyl]-4-(1-methylethyl)-, (4S)- (9CI) (CA INDEX NAME)

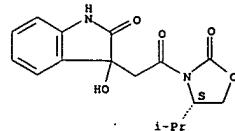
Absolute stereochemistry.

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
 ACCESSION NUMBER: 2005:811739 CAPLUS  
 DOCUMENT NUMBER: 143:229863  
 TITLE: A manufacturing of (triazolylmethyl)indole derivatives  
 INVENTOR(S): and their intermediates Martin, Pierre; Berens, Ulrich; Boudier, Andreas; Dosenbach, Oliver  
 PATENT ASSIGNEE(S): Ratiopharm G.m.b.H., Germany  
 SOURCE: PCT Int. Appl. 67 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005075422	A1	20050818	WO 2005-EP793	200505127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				
CA 2553652	A1	20050818	CA 2005-2553652	20050127
EP 1751104	A1	20070214	EP 2005-707035	20050127
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			EP 2004-100303	A 20040128
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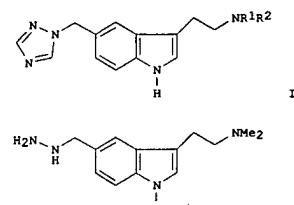
OTHER SOURCE(S): MARPAT 143:229863  
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L3 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

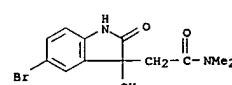


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

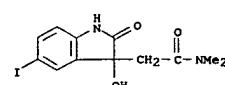
L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB The invention relates to a preparation of (triazolylmethyl)indole derivs. of formula I (wherein: R1 and R2 are independently H or alkyl) and their intermediates. For instance, anti-migraine agent rizatriptan I [R1 = R2 = Me; no biol. data] was prepared from [(hydrazinomethylindolyl)ethyl]-dimethyl-amine II with a yield of 55%.  
 IT 717139-78-1P 717139-81-6P 717139-87-2P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (manufacturing of (triazolylmethyl)indole derivs. and their intermediates)  
 RN 717139-78-1 CAPLUS  
 CN 1H-Indole-3-acetamide, 5-bromo-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-(9CI) (CA INDEX NAME)

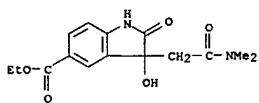


RN 717139-81-6 CAPLUS  
 CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-iodo-N,N-dimethyl-2-oxo-(9CI) (CA INDEX NAME)



RN 717139-87-2 CAPLUS  
 CN 1H-Indole-3-carboxylic acid, 2,3-dihydro-3-hydroxy-5-iodo-N,N-dimethyl-2-oxo-(9CI) (CA INDEX NAME)

L3 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
3-hydroxy-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



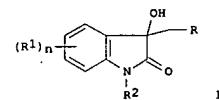
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2004:546477 CAPLUS  
DOCUMENT NUMBER: 141:89009  
TITLE: Synthesis of tryptamine derivatives and intermediates thereof  
INVENTOR(S): Berens, Ulrich; Dosenbach, Oliver; Sprenger, Daniel  
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.  
SOURCE: PCT Int. Appl., 84 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056769	A2	20040708	WO 2003-EP50992	20031212
WO 2004056769	A3	20040916		
WO 2004056769	B1	20041104		
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RW: BW, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TZ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,				
TG				
CA 2508290	A1	20040708	CA 2003-2508290	20031212
AU 2003299227	A1	20040714	AU 2003-299227	20031212
EP 1572647	A2	20050914	EP 2003-798460	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, NL, LU, MU, SE, NC, PT, IE, SI, LT, LV, FI, RO, MK, CY, IL, TR, BG, CZ, EE, HU, SK				
CN 1729174	A	20060201	CN 2003-80107086	20031212
JP 2006516128	T	20060623	JP 2004-561492	20031212
US 2006058367	A1	20060316	US 2005-539151	20050616
PRIORITY APPLN. INFO.:				
WO 2003-EP50992				A 20021220
				W 20031212

OTHER SOURCE(S): MARPAT 141:89009

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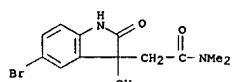


L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

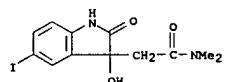
AB Indoleacetates I [R = CO2R3; R1 = (un)substituted alkyl, aryl, heterocyclic, alkylsulfonyl, OH, SH, NO2, halogen, CN, CONH2, CONHNH2, CO2H, alkenyl, alkynyl, cycloalkyl, acyloxy, NH2, NHHN2, B(OH)2; R2 = H, (un)substituted alkyl, CO2H, alkylsulfonyl, alkylsulfonyl, aryl, CONH2, silyl; R3 = (un)substituted alkyl; n = 0-4] were prepared and converted to I [R = CONR4R5; R4, R5 = (un)substituted alkylene] which were in turn converted to indoleacetamides and tryptamines. The synthesis methods and products are useful in the synthesis of pharmaceuticals. Thus, 5-bromoindat was treated with CH2(CO2H)2 and ClCONMe2 to give I [R = CONMe2, R1 = 5-Br, R2 = H] which was treated with BF3·Et2O and BH3·Me2SO to give 2-(5-bromo-1H-indol-3-yl)-N,N-dimethylacetamide or with BF3·Et2O and NaBH4 to give 2-[2-(5-bromo-1H-indol-3-yl)ethyl]-N,N-dimethylacetamide.

IT 717139-78-1P 717139-81-6P 717139-88-3P  
717139-92-9P 717139-93-0P 717139-95-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); (preparation of tryptamine derivs. and intermediates thereof)

RN 717139-78-1 CAPLUS  
CN 1H-Indole-3-acetamide, 5-bromo-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-(9CI) (CA INDEX NAME)

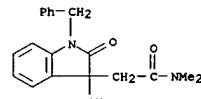


RN 717139-81-6 CAPLUS  
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-iodo-N,N-dimethyl-2-oxo-(9CI) (CA INDEX NAME)

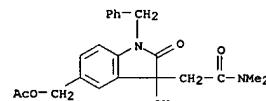


RN 717139-88-3 CAPLUS  
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

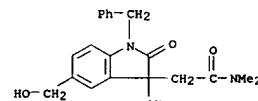
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



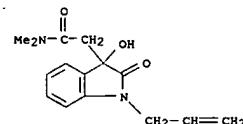
RN 717139-92-9 CAPLUS  
CN 1H-Indole-3-acetamide, 5-[(acetyloxy)methyl]-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 717139-93-0 CAPLUS  
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-(hydroxymethyl)-N,N-dimethyl-2-oxo-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



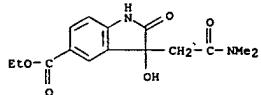
RN 717139-95-2 CAPLUS  
CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-(2-propenyl)- (9CI) (CA INDEX NAME)



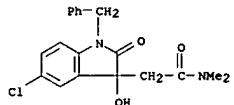
IT 717139-87-2P 717139-91-8P 717139-94-1P  
717139-96-3P  
RL: SPN (Synthetic preparation); PREP (Preparation); (preparation of tryptamine derivs. and intermediates thereof)

RN 717139-87-2 CAPLUS

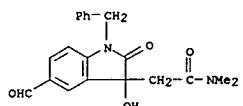
L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)  
 CN 1H-Indole-5-carboxylic acid,  
 3-[2-(dimethylamino)-2-oxoethyl]-2,3-dihydro-  
 3-hydroxy-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 717139-91-8 CAPLUS  
 CN 1H-Indole-3-acetamide,  
 5-chloro-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-  
 (phenylmethyl)- (9CI) (CA INDEX NAME)



RN 717139-94-1 CAPLUS  
 CN 1H-Indole-3-acetamide,  
 5-formyl-2,3-dihydro-3-hydroxy-N,N-dimethyl-2-oxo-1-  
 (phenylmethyl)- (9CI) (CA INDEX NAME)



RN 717139-96-3 CAPLUS  
 CN 1H-Indole-3-acetamide, 2,3-dihydro-3-hydroxy-5-(hydroxymethyl)-N,N-  
 dimethyl-2-oxo-1-(2-propenyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

